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Title: Workshops on Efficient Use of Scientific Computing

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INFORMAL WORKSHOP PROCEEDINGS

WORKSHOPS ON EFFICIENT USE OF SCIENTIFIC COMPUTING

Ben Noble, August 2, '91.

1. Background and summary.

Two 2-day workshops were held. These concentrated on MATLAB, which is a high-level computer language for scientific and engineering calculations. It is extremely useful for many exploratory investigations, and for problems that need efficient use of matrices.

Some of the advantages of MATLAB over lower-level languages like FORTRAN are:

- The essentials can be learned very easily - one day.
- Programs tend to be short, easy to write and read.
- MATLAB is interactive, which makes it easy to debug and make changes in programs.
- Excellent, easy-to-use graphics.
- Tedious aspects of lower-level languages are eliminated.

The work performed under the contract can be summarized as follows:

1. In the summer of '90, a Brunel University graduate student (Gudrun Schmidt) wrote a Master's degree dissertation entitled "Finite element programs using MATLAB", partly supported by the contract. This is discussed further in Section 4, below.

2. Material was prepared and presented at a workshop held at the US Army, ARD & E Center (Benet Lab), Watervliet, NY, which took place on Nov. 15-16 (Contact: Dr John Vasilakis.) This is discussed in Section 2, below.

3. Further material was prepared and presented at a second workshop, at the US Army R & D Center, Natick, Mass., which took place on May 22-23, '91. (Contact: Dr Louis Piscitelle.) This is discussed in Section 3, below.

An interesting side-development was that Dr Julian Wu of the US Army Research Office, ARO, and myself visited MATHWORKS and talked at some length to Dr Cleve Moler, who is the genius responsible for inventing MATLAB.

Dr Wu has copies of the material discussed below.

2. The first workshop, at the Benet Lab., Watervliet, Nov. '90.

There were 22 participants, drawn from various US Army labs. Because of this number, the workshop consisted of mainly lecture/discussion sessions, with some time devoted to "hands-on" computer work. The facilities available were excellently organized by Dr Vasilakis.

The schedule was as follows for the lectures, the remaining time being available for computer work.

FIRST DAY:

1. Introduction.
2. MATLAB basics.
3. MATLAB matrix programs, with math. background.

SECOND DAY:

4. MATLAB toolboxes.
5. Further examples.
6. Finite-element programs, including time-dependence.

The literature provided was a copy of 100+ pages of handwritten transparencies used in the workshop. These consisted of the following sections:

1. Introductory remarks and general information.
2. MATLAB basics.
3. MATLAB matrix functions.
4. MATLAB toolbox functions.
5. Some illustrative MATLAB programs.
6. Examples from the Schmidt dissertation. This was accompanied by a computer disk from the thesis.

A questionnaire was circulated at the end of the workshop, which produced constructive suggestions, and indicated a positive response to the workshop.

3. The second workshop, at the Natick lab., Mass., May, '91.

This was organized quite differently from the first workshop, mainly because a smaller number of participants (10) were involved, from within the same section of the one lab. The credit for the change in organization goes to Dr Piscitellei.

In addition to copies of the transparencies from the first workshop, and a copy of the Schmidt finite-element programs, the following were provided:

1. Extra written material including MATLAB examples covering diverse topics such as zeros of functions, rank of a matrix, oscillations (eigenvalues), reconstruction of images (singular values), nonlinear oscillations and bifurcation, electrical

cicuits, electromagnetic theory, etc.

2. An experimental set of four interactive tutorials on MATLAB basics. These were well received.

3. A pretty miscellaneous set of MATLAB programs of general interest.

4. A set of about 50 MATLAB programs produced by Profeesor Howard Wilson, Mechanical Eng. Dept., University of Alabama, a subset of these being selected for particular attention at this workshop.

The first day of this second workshop was devoted to a rapid introduction to MATLAB. By that time the participants decided that they knew enough to launch into projects of their own choosing. The second day was devoted to these projects. The two most memorable to me are visualizing graphically the motion of a curve in three dimensions, and using the MATLAB solvers for initial-value ODE problems to solve boundary-value problems.

This method of organizing the workshop worked out well, as a questionnaire indicated. For further comments see Section 5.

4. The Schmidt dissertation on finite-element methods for PDE's.

This was a quite remarkable effort on the part of the student, who had little previous experience of computing at this level.

This 90-page dissertation consists of three parts, each containing several MATLAB programs (25 in all):

Part 1. The Laplace and Poisson equations..
Part 2. Two-dimensional elasticity.
Part 3. Time-dependent problems - heat conduct. & Burger's.

The main reason for not circulating this dissertation more widely is that MATHWORKS are releasing a toolbox on sparse matrices this autumn. The programs in the dissertation need some modification to take advantage of this and other points arising from the dissertation. This will be done when the MATLAB sparse matrix package is released. It would be a mistake to make these PDE programs generally available too early. Since they can form the basis for much future work, we wish to ensure that they are made as good as possible, in view of recent developments.

5. Concluding remarks.

On the basis of the above experience, my personal feeling about the best way to run workshops on a fairly specialist (though important) topic like MATLAB, with a single instructor, is the following. For the sake of clarity I describe two extremes. Then a third which is a combination of both.

• If one has perhaps 10/15 participants who can be subdivided into groups of research or development scientists, each consisting of 1 - 4 members, with computing experience and an interest in different specific problems, one can run a successful 2-day workshop as at Natick. The first day would be devoted to a general introduction to MATLAB, pointing people in the right direction for the second day that would be devoted to work on their specific problems. This is comparatively easy to organize at a single lab like Natick. It would be more difficult, but not impossible, if participants came from different labs.

• The second situation is that there are a larger number of participants, most of whom attend for general information, as at the Benet lab workshop. Once the interactive MATLAB tutorials are developed in a definitive form (see Section 3, point 2, above), it will be much easier to do this, since the participants need spend only enough time at terminals to ensure that they can use the tutorials at their leisure at the end of the workshop.

• In an ideal world one can visualize a third possibility. The workshop could last a week. The first two days would be general information (including computer symbol manipulation). Those interested in general information only would depart, but those with specific problems would remain for the rest of the week. This is probably too much for a single instructor. I am too old to initiate such an effort, but I would be interested in taking an active part if one were established.

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